# MCNPX, VERSION 2.5.f

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February 23, 2005

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## MCNPX, VERSION 2.5.f

### **ABSTRACT**

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. The new capabilities of the latest version, MCNPX 2.5.f, are described.

### 1.0. INTRODUCTION

MCNPX (MCNP eXtended) is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed; it can be used with confidence. Major MCNPX versions, such as MCNPX 2.4.0, are available from the Radiation Safety Information and Computational Center (RSICC, <a href="http://www-rsicc.ornl.gov">http://www-rsicc.ornl.gov</a>) and the Office of Economic Community Development (OECD)/Nuclear Energy Agency (NEA) (<a href="http://www.nea.fr/">http://www.nea.fr/</a>). For approved users, beta test program versions, including MCNPX2.5.f, may be downloaded from the MCNPX website at <a href="http://mcnpx.lanl.gov/">http://mcnpx.lanl.gov/</a>.

Complete documentation of MCNPX features beyond MCNPX2.3.0 and MCNP4C is provided in "MCNPX Extensions, Version 2.5.0," available on the Worldwide Web at http://mcnpx.lanl.gov/opendocs/reports/Interface.doc.

## 1.1. New MCNPX 2.5.f Capabilities

MCNPX 2.5.f offers many new capabilities. The complete summary of MCNPX capabilities beyond MCNPX 2.3.0 and MCNP4C is provided in the MCNPX features list available on the MCNPX website at <a href="http://mcnpx.lanl.gov/">http://mcnpx.lanl.gov/</a>. The new capabilities and enhancements of MCNPX 2.5.f beyond MCNPX 2.5.e are listed as follows (where applicable, the initials of the principal developers are shown in parentheses).\*

- Mesh Tally Plots without Auxiliary Codes (JSH/GWM)
- Pulse-Height Tally (PHT) with Variance Reduction (JSH/GWM)
- Windows Intel Compiler Support (GWM)
- Corrections/Enhancements /Extensions
  - o Improved Photonuclear Model Data (FXG)
  - o FT8 Capture Tallies with Time Gating (JSH)
  - o User Specification of Multiplicity Constants—FMULT (JSH)
  - o New Spontaneous Fission Multiplicity Data (JSH)
  - o Correction for Fission Multiplicity Negative Gaussian Tail Bias (JSH)

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- o Translated Sources Can Have Dependence (FXG/GWM)
- o Plot Pause Command Interrupts (JSH)

#### 1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay \$20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. European users are awarded €20. We also will pay a brand new \$2 bill for any error in MCNPX that has been inherited from its constituent codes.\*

MCNPX is a better-quality code than MCNP4C3. First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors, and most of those awards have been given for problems carrying over from older code versions; very few errors have been found in the new MCNPX versions. A listing of winners is available at <a href="http://mcnpx.lanl.gov/">http://mcnpx.lanl.gov/</a>. MCNPX bugs are described in the release notes for each MCNPX version.

### 1.3. Availability

MCNPX 2.4.0 is available from the RSICC in Oak Ridge, Tennessee, USA, at <a href="http://www-rsicc.ornl.gov/">http://www-rsicc.ornl.gov/</a>. MCNPX 2.4.0 is also available from the OECD NEA Data Bank in Paris, France, at <a href="http://www.nea.fr/">http://www.nea.fr/</a>.

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA, it is made available to more than 1500 MCNPX beta testers worldwide. MCNPX 2.5.f is available to beta testers on the MCNPX website at <a href="http://mcnpx.lanl.gov/">http://mcnpx.lanl.gov/</a>. To apply for a beta test password and have access to the latest MCNPX versions, contact mcnpx@lanl.gov.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

### 2.0. DESCRIPTION OF NEW MCNPX 2.5.f FEATURES

The principal new capabilities of MCNPX 2.5.F are

- mesh tally plots without auxiliary codes (JSH/GWM),
- PHTs with variance reduction (JSH/GWM), and
- Windows Intel support (GWM).

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<sup>\*</sup> Cash Award Fine Print: This offer is subject to cancellation or modification without notice. A bug is defined as an error we choose to correct in the source code. We make awards even for the most trivial or insignificant of problems, but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We endeavor to make MCNPX the most error-free and robust Monte Carlo radiation transport code possible, and we back this code with a cash guarantee.

# 2.1. Mesh Tally Plots

Tally output, including mesh tallies, radiography tallies, and lattice tallies, now may be plotted as two-dimensional color contour plots. Mesh tallies also can be plotted as superimposed over problem geometries.

The following combinations are available:

Postprocessing, MCNPX Z option, RMCTAL=<mctal filename> Mesh tallies, radiography tallies, lattice tallies, and all other tallies

Postprocessing, MCNPX Z option, RUNTPE=<runtpe filename>
Radiography tallies, lattice tallies, and all other tallies
In the PLOT mode mesh tally contours superimposed over problem geometries

Run-time plotting: all of the above combinations are available during a run with the MPLOT input file card.

## **2.1.1.** Example

Figure 1 shows a mesh tally of critical configuration of seven identical barrels of fissionable material.

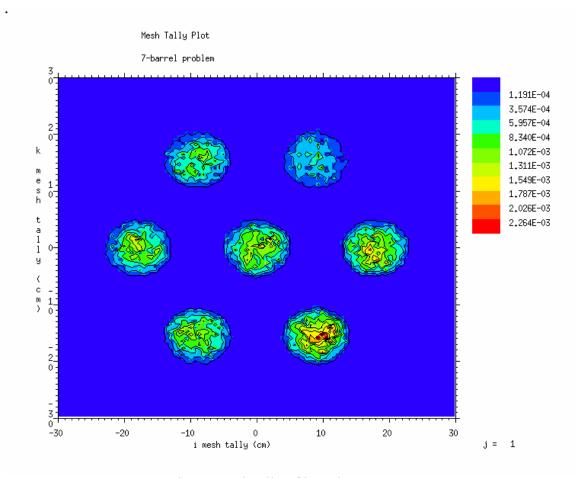


Fig. 1. Mesh tally of barrel geometry.

## The input file for this problem is

```
cylinders containing critical fluid in macrobody hex lattice
1 1 -8.4
                              imp:n=1
              -1
                       u=1
2 0
              -2
                              imp:n=1
                       u=1
3 \ 2 \ -2.7
                              imp:n=1
              -3 1 2 u=1
4 3 -.001
               3
                       u=1
                              imp:n=1
10 3 -.001
              -6 lat=2 u=2
                              imp:n=1 fill=-2:2 -2:2 0:0
                                       2 2 2 2 2
                                       2 2 1 1 2
                                      2 1 1 1 2
                                      2 1 1 2 2
                                       2 2 2 2 2
11 0
              -8
                              imp:n=1 fill=2
50 0
               8
                              imp:n=0
              0 12 0
1 rcc 0 0 0
2 rcc 0 12 0
              0 8
                       5
                   0
              0 22 0
3 rcc 0 -1 0
                       6
6 rhp 0 -1 0
              0 22 0
                       9 0 0
8 rcc 0 -1 0
              0 22 0
      1001 5.7058e-2
                        8016 3.2929e-2
m1
```

```
92238 2.0909e-3 92235 1.0889e-4
    13027 1
m2
    7014 .8 8016 .2
m3
С
fc14 total keff in each element
f4:n (1<10[-2:2 -2:2 0:0]<11)
fq4 f m
sd4 1 24r
f14:n (1<10[-1 1 0]) (1<10[0 1 0])
      (1<10[-1 0 0]) (1<10[0 0 0]) (1<10[1 0 0])
       (1<10[0 -1 0]) (1<10[1 -1 0]) t
fq14 f m
sd14 1 7r
tf14 4
fm14 (-1 1 -6 -7)
print -160
prdmp 2j 1
kcode 1000 1 10 50
ksrc 0 6 0 18 6 0 -18 6 0 9 6 15 -9 6 15 9 6 -15 -9 6 -15
tmesh
rmesh12
cora12 -30. 99i 30.
corb12 0.12.
corc12 -30. 99i 30.
endmd
```

The plot command is

mcplot> tal 12 free ik .

The geometry is shown in Fig. 2.

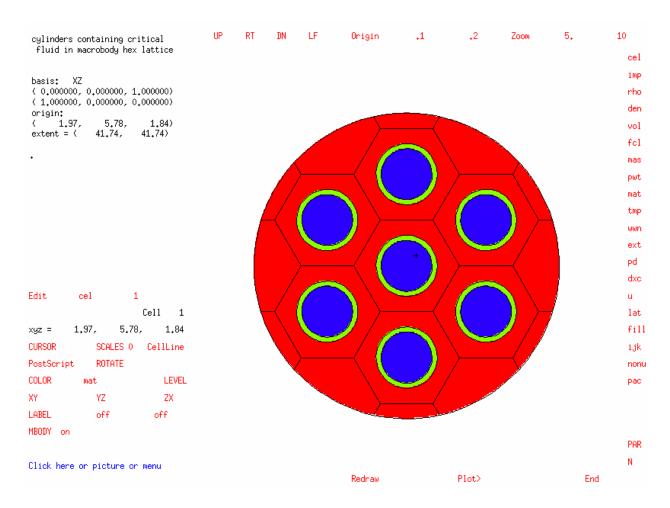


Fig. 2. Geometry of the seven-barrel problem.

Figure 3 shows the mesh plot superimposed over the geometry plot. The MCNPX Z option is used, and the commands are

```
MCPLOT> RUNTPE=<runtpe filename>
MCPLOT> PLOT
PLOT> py 4 ex 40 or 0 4 0 la 0 1 tal12 color on la 0 0 con 0 100 % .
```

After the PLOT command, the MCNPX interactive geometry plotter pops up. If the PLOT> button (bottom center) is clicked, then the above command after the PLOT> prompt can be entered. Alternatively, the mesh tally superimposed on the geometry can be viewed by clicking buttons of the interactive tally plot. These options are described later in Section 2.1.3.

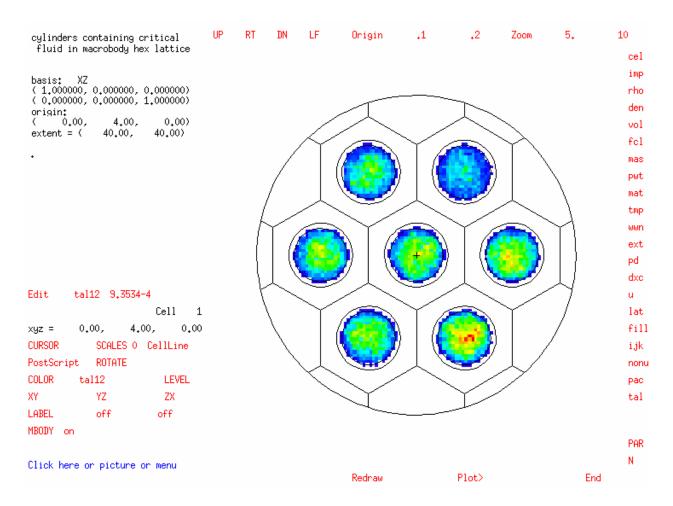


Fig. 3. Mesh plot superimposed on geometry plot.

Note that each outer barrel is expected to have the same source and flux distributions and that the center barrel should have a higher value. However, the mesh tally shows that the barrels do not have the expected distribution. The asymmetric distribution is a known Monte Carlo deficiency and arises in all Monte Carlo codes, including MCNP4C, MCNP5, and MCNPX: eigenvector fluxes generally are falsely converged in eigenvalue problems of critical systems. It is evident that the mesh tally is useful in assessing such deficiencies.

### 2.1.2. User Interface for Contour Tally Plots

Mesh tally and other contour plots may use all of the usual MCNPX tally plot (MCPLOT) commands. Mesh tallies can be plotted only from MCTAL files in the tally plotter and can be plotted only from RUNTPE files in the geometry plotter (see Section 2.1.3). Radiography, lattice, and other contour plots can use either MCTAL or RUNTPE files but can be plotted only in the tally plotter and not superimposed over geometries in the geometry plotter.

The FREE and CONTOUR commands have the following extensions.

#### 2.1.2.1. Free Command

The MCPLOT free command is

```
FREE X[Y] [nxm] [all] [noall] .
```

For mesh tallies,

FREE ij

FREE *jk* 

FREE ik

are used, where *i,j,k* refer to the CORA, CORB, and CORC mesh tally dimensions.

For radiography tallies,

is used to make a contour plot of the s- and t- radiography axes.

For lattice tallies, i,j,k, refer to the i,j,k lattice indices.

If the lattice is fully specified, e.g.,

```
fill=-2:2 -2:2 0:0
2 2 2 2 2
2 2 1 1 2
```

2 1 1 1 2

2 1 1 2 2 2 2 2 2 2

then the [nxm] entries are not needed. If the lattice is not fully specified, e.g.,

```
fil1=2 ,
```

then the i and j dimensions must be given with the [nxm] entries, e.g.,

FREE 
$$ik$$
 20x10 FIX  $j=15$ .

The FIX command has its usual meaning, namely that the j=15 slice of the full i,j,k lattice will be used.

The "all" and "noall" keywords specify if the minimum and maximum contour range should be taken from all of the tally bins ("all") or just from those of the FIXED command slice ("noall"—default).

One-dimensional mesh, radiography, and lattice tallies are also possible simply by giving the free dimension on the FREE command:

FREE 
$$i$$
 FIXED  $j=10$   $k=12$ .

Again, for lattice tallies that are not fully specified, the [mxn] dimensions must be provided. Mesh and radiography tallies are always fully specified, so [mxn] is never required for them.

#### 2.1.2.2. Contour Command

The MCPLOT contour command is

```
CONTOUR [cmin cmax cstep] [command] [command] .
```

All entries are optional. The [cmin cmax cstep] entries are the minimum, maximum, and step values for contours. The [cmin cmax cstep] entries are numbers and must appear together. The other commands may appear anywhere after the CONTOUR command and are

```
%
         interpret step values as percentages. The default is 5 95 10 %:
         interpret step values as percentages. The default is 5 95 10 %;
pct
         interpret step values as absolute values of contour levels;
lin
         contour levels logarithmically spaced between cmin and cmax, with cstep values in
log
         between;
         contours normalized to min and max values of entire tally;
all
         contours normalized to min and max values of (FIXED command) contour slice:
noall
         draw lines around contours (default);
line
         do not draw lines around contours:
noline
color
         make color contour plot (default);
nocolor no color; draw line contours only.
```

## Examples:

```
CONTOUR 5 95 10 % line color
```

Ten contour lines will be at 5%, 15%, ..., 95% of the maximum value. Lines will be drawn around the colored contours, as shown in Fig. 1. This is the default setting.

```
CONTOUR 1e-4 1e-2 12 log .
```

Twelve contour lines will be logarithmically spaced between tally values of 1e-4 and 1e-5.

## 2.1.3. User Interface for Mesh Tallies Superimposed on Geometry Plots

Mesh tallies also may be superimposed over geometry plots in the geometry plotter using RUNTPE files. Mesh tally plots may be superimposed over geometry plots either while a run is progressing (MPLOT card) or at the end of a run (MCNPX Z option).

## 2.1.3.1. Accessing Superimposed Mesh Tallies

Mesh tallies can be superimposed over geometry plots in two ways.

During the course of a calculation, an MPLOT card in the INP file can be used to plot the mesh tallies. The plot of Fig. 3 would be achieved with the following MPLOT card:

```
mplot freq 3000 plot ex 40 py 4 la 0 1 tal12.1 color on la 0 0
```

```
cont 0 100 pct
```

The "freq 3000" command causes a plot to be made every 3000 histories. The "plot" command then transfers plotting from the tally plotter to the geometry plotter. The remaining commands are described in Section 2.1.3.2.

When a calculation is completed, the mesh tallies may be plotted as superimposed over geometries using the MCNPX Z option. Only RUNTPE files can be used; MCPLOT files cannot be used because they do not contain the geometry information. The RUNTPE file may be specified either in the execution line,

```
MCNPX Z RUN=<runtpe filename>,
```

or the RUNTPE file may be specified in the usual way anytime while doing tally plots:

```
MCNPX Z mcplot> run=<runtpe filename>
```

Then to get the mesh tallies, the geometry plot mode must be requested:

```
mcplot> PLOT .
```

At this time, the interactive geometry plotter screen will pop up and commands may be entered either interactively or in command mode by striking the PLOT> button in the bottom center of the screen.

## 2.1.3.2. *Commands*

First, the geometry must be specified in the usual manner. For the geometry of Fig. 2, the plot commands are

```
PLOT> or 0 4 0 py 4 ex 40 la 0 0 .
```

The same geometry can be viewed by using the Zoom, Origin, XZ, and LABEL interactive buttons.

Next, the tally must be selected as the "Edit" quantity. In the command mode, the only way to do this is to select the tally as the label quantity, transfer the label to the color quantity, and then turn the labels back off:

```
PLOT> la 0 1 tal12.1 color on la 0 0 .
```

Note that only mesh tallies will be recognized. If there are multiple mesh tally bins, e.g.,

```
rmesh11:h flux popul
```

then the number after the decimal indicates which bin. In this case, tall 1.1 refers to the "flux" mesh tally and tall 1.2 refers to the "popul" mesh tally.

PLOT>

or

Interactive plot buttons can be used to achieve the same result. First, the mesh tallies must be made the edit quantity by clicking the last of the buttons in the far right column of the screen.

Click	tal	(make mesh tallies the edit quantity)
Click	N	(cycle through available mesh tally numbers)
Click	IP	(cycle through mesh tally bins)

The edit quantity, e.g., tal12.1, now has been specified. Next, change the color parameter (default = "mat"), by clicking COLOR twice.

Click	COLOR	(will change "mat" to "off")
Click	COLOR	(will change "off" to the edit quantity, "tal12.1")
Click	Redraw	(bottom center button – to make new picture)

Two other commands are also useful: meshpl and contour.

The actual mesh tally grid can be displayed by clicking "CellLine" and cycling through the options to get either "MeshTaly" (draws mesh tally grid lines over plot) or "MT+Cell" (draws mesh tally grid lines and cell surface lines over plot). In the command prompt mode, this is done with

```
meshpl = 6
                     (mesh tally grid lines)
```

```
meshpl = 7
PLOT>
                                  (mesh tally grid lines plus cell surface lines).
```

The contour levels can be adjusted using the contour command. No interactive button is available for this, so to get from interactive to command mode, either the "Click here or picture or menu" (bottom left of interactive screen) or "PLOT>" (bottom center) must be struck. The contour command is

```
CONTOUR
           cmin cmax [cstep] command.
```

The "cmin cmax cstep" entries are the minimum, maximum, and step values for contours. Superimposed geometry mesh tally plots do not use steps: the values are shaded by 64 colors. Thus, the estep entry is ignored and can be omitted; it is allowed only for consistency with the CONTOUR command in the tally plotter (Section 2.1.2.2). The "cmin cmax cstep" entries are numbers and must appear together. Once a CONTOUR command is entered, subsequent CONTOUR commands use the previous "cmin cmax estep" values; thus, only the "command" entry is required. The "command" entry may appear before cmin or after estep or by itself. "CONTOUR" may be abbreviated to simply "CON" or "CONT". The allowable entries for "command" are

```
%
         interpret step values as percentages. The default is 5 95 10 %;
         interpret step values as percentages. The default is 5 95 10 %;
pct
```

lin interpret step values as absolute values of contour levels; log contour levels logarithmically spaced between cmin and cmax; off use default: 0 100 %

The remaining command options for tally plots ("all", "noall", "line", "noline", "color", and "nocolor" (Section 2.1.2.2) make no sense for geometry mesh tally plots and are disallowed. Some examples are

```
cont 0 100 pct
con 5 95 10 %
contour off
cont 1E-4 2 log
```

## 2.1.4. Other Notes and Future Work

A consequence of the new mesh tally contour plotting capability is that MDATA files are ignored in continue runs. MDATA files and the auxiliary GRIDCONV code still are supported for plotting of mesh tallies with other postprocessors, such as MORITZ and TECPLOT. A new MDATA file is written at the end of each initial or continue run.

When using COMMAND files (which use a preselected sequence of MCPLOT tally plot commands) the "RETURN" command must follow geometry plot commands to revert from the geometry plotter back to the tally plotter.

The future work is as follows:

- 1. Treat the mesh tallies as regular tallies. Among the many consequences are
  - cleaner code;
  - RMESH, CORA, CORB, CORC, etc., could be anywhere in the input deck (TMESH and ENDMD would be ignored) and all other tally features, such as FM, DE, DF, FC, CF, SF, FU, FT, E, T, EM, and TM, would be enabled and consistent with other tallies; and
  - tally plot mesh tallies (Section 2.1.2) could use RUNTPE files and not be limited to MCTAL files.
- 2. Plot theta and phi values from cylindrical and spherical meshes correctly in tally plots and plot spherical mesh tally grid lines in geometry plots.

# 2.2. Pulse-Height Tallies with Variance Reduction

Until now, variance reduction techniques (VRTs) have not been compatible with F8 PHTs. Unlike standard Monte Carlo tallies, which score events as they occur, PHTs combine the energy deposition of many events in a single Monte Carlo "history." The entire history tree must score, not just a single event in the tree. Further, VRT events such as Russian roulette can kill the entire tree if they occur after a physical event such as photon pair production.

A new method has been developed that enables VRTs with PHTs.\* Results are very problem dependent, and variance reduction is more challenging than with other MCNPX tallies. On a space satellite problem, calculations were sped up by two orders of magnitude.† Although the new capability greatly enhances most F8 PHT calculations, it has not been extended to all VRTs or physics combinations. See "Future Work" below.

No new user interface changes are required. If VRTs are used with PHTs, a fatal error no longer occurs unless the VRTs are incompatible with PHTs. Several new warning messages occur if it appears that the VRTs will be inefficient with PHTs.

#### 2.2.1. Future Work

PHTs work with VRTs in the most widely used F8 PHT application: electrons and photons. They do not work with other particle types and have other extensions that will have to await further funding. Among these future work items are

- enable neutrons and other particles to use VRTs with PHTs;
- enable more than a single F8 tally per problem;
- enable DXTRAN and SPABI VRTs; and
- extend to FT special treatments, particularly the light tally with anticoincidence, residual nuclei, and capture options (FT PHL, RES, and CAP options).

## 2.3. Windows Intel Compiler

Until now, MCNPX PC versions required compilation with the Compaq Digital Fortran (CDF) or earlier Digital Visual Fortran (DVF) Fortran90 compilers. Now the Intel Fortran compiler can be used.

The Intel executable runs the MCNPX test suite an average of 24% faster than the CVF executable. Therefore, the Intel compiler is the new default for compilation with Windows PC.

The four configure options on Windows are

Configure (Build with the Intel compiler)
Configure CVF (Build with the CVF compiler)
Configure I8 (Build with 8-byte integers)
Configure MPI (Build the MPI version)

-

<sup>\*</sup> John S. Hendricks and Gregg W. McKinney, "Pulse-Height Tallies with Variance Reduction," Los Alamos National Laboratory report LA-UR-04-8431 (2004).

<sup>&</sup>lt;sup>†</sup> John S. Hendricks and Jane M. Burward-Hoy, "Monte Carlo Radiation Detector Modeling in Space Systems," Los Alamos National Laboratory report LA-UR-05-0278 (2005).

### 3.0. MCNPX 2.5.f FEATURE EXTENSIONS AND ENHANCEMENTS

Several MCNPX features have been extended and have included changes or additions to the user interface:

- improved photonuclear modeling (FXG),
- FT8 capture tallies with time gating (JSH),
- user specification of multiplicity constants—FMULT (JSH),
- new spontaneous fission multiplicity data (JSH),
- correct for fission multiplicity negative Gaussian tail bias (JSH),
- translated sources can have dependence (FXG/GWM),
- plot pause command interrupts (JSH),
- PTRAC for N-particles (GWM),
- DXTRAN / detectors with model physics (isotropic approximation) (GWM), and
- additional enhancements.

## 3.1. Improved Photonuclear Modeling

The threshold for photonuclear reactions is now 1 MeV.

The GDR.DAT data file has been improved by better fits of the parameters for thorium, uranium, and plutonium isotopes based on data from the Russian BOFOD library. The extended list of tabulated wam parameters for thorium, uranium, and plutonium isotopes corrects the fission probability calculated in the routine set\_wam.F within CEM2k. Also, an improved fit of photoabsorption cross sections in the updated CEM2k pnxs.F routine occurs based on experimental data from Muccifora, Bianchi, Brookes, Michalowski, and Chollet.

## 3.2. FT8 Capture Tallies with Time Gating

The coincidence capture tally now allows specification of pre-delay and gate width\* with the "gate" keyword on the FT8 card. The "gate" keyword may appear anywhere after the "cap" keyword and is part of the "cap" command. Immediately following the "gate" keyword must be the predelay time and the total gate width, both in units of shakes (1.0e-8 seconds).

The addition of the pre-delay and time gate width changes the capture tally scoring. When a neutron is captured at time t0 in the specified cell by the specified nuclide (22 and  ${}^{3}\text{He} = 2003$  in all three tallies below) the gate is "turned on." If the pre-delay is t1 and the gate width is t2, then all captures between t0 + t1 and t0 + t1 + t2 are counted. For a history with no captures, no events are scored. With one capture, 0 events are scored. With two captures, the first turns on the time gate are at time t0 and scores 0; the second will score one event if it is captured between between t0 + t1 and t0 + t1 + t2 or score another 0 if outside the gate.

<sup>\*</sup>Martyn T. Swinhoe, John S. Hendricks, and Douglas R. Mayo, "MCNPX for Neutron Multiplicity Detector Simulation," Los Alamos National Laboratory report LA-UR-04-8025 (2004).

Other entries after the "cap" keyword are the same but now may be placed in a more flexible order, as shown in the following examples. The negative entries change the allowed number of captures and moments (defaults 21 and 12 are changed to 40 and 40 in F78 below). The list of capture nuclides ( ${}^{3}\text{He} = 2003$  in all three tallies below) may also be anywhere after "cap."

Examples for the three capture tallies above now follow. The capture tally without gating (f18) is unchanged from MCNPX 2.5.E. An infinite gate (F38) results in a very different Print Table 118: the number of captures is the same, but the moments are offset by one. A finite gate (F78) has fewer captures, as expected.

Example 1: Capture Tally without Gate

#### Input:

```
f18:n 22
ft18 cap 2003
```

### Output:

```
neutron captures, moments and multiplicity distributions. tally
                                                                                     18
print table 118
 weight normalization by source histories =
                                                      20000
 cell:
neutron captures on 3he
                                                    multiplicity fractions
                        captures
                                     captures
            histories by number
                                   by weight
                                                  by number
                                                                by weight
                                                                              error
 captures = 0 13448
                           0
                               0.00000E+00 6.72400E-01 6.72400E-01
                                                                             0.0049
                                                6./2400E - 01
 captures = 1 5550
captures = 2 588
                       5550 2.77500E-01
1176 5.88000E-02
                                                              2.77500E-01
                                                                             0.0114
                                                2.94000E-02
                                                              2.94000E-02
                                                                             0.0406
                 238 714
94 376
40 200
26 156
                 238
captures = 3
                                3.57000E-02
                                                1.19000E-02 1.19000E-02
                                                                             0.0644
captures = 4
captures = 5
captures = 6
                                                              4.70000E-03
                                1.88000E-02
                                                4.70000E-03
                                                                             0.1029
                                 1.00000E-02
                                                              2.00000E-03
                                                2.00000E-03
                                                                             0.1580
                                 7.80000E-03
                                                              1.30000E-03
                                                1.30000E-03
                                                                             0.1960
 captures = 7
                  8 56 2.80000E-03
5 40 2.00000E-03
1 9 4.50000E-04
                                                4.00000E-04
                                                              4.00000E-04
                                                                             0.3535
captures = 8
captures = 9
                          40
                                2.00000E-03
4.50000E-04
                                                2.50000E-04
                                                              2.50000E-04
                                                                             0.4472
                                                5.00000E-05
                                                              5.00000E-05
                    1
                                                                             1.0000
 captures = 12
                          12 6.00000E-04
                                                5.00000E-05 5.00000E-05
                                                                             1.0000
                         16 8.00000E-04
                                               5.00000E-05
                                                              5.00000E-05
 captures = 16
                    1
                                                                             1.0000
    total
                20000
                         8305 4.15250E-01 1.00000E+00
                                                              1.00000E+00
                                                                             0.0128
      factorial moments
                                      by number
                                                              by weight
                                4.15250E-01 0.0128
                                                         4.15250E-01 0.0128
             3he
    3he(3he-1)(3he-2)/3!
                                1.59300E-01 0.0651
                                                         1.59300E-01 0.0651
                                1.47900E-01 0.2165
                                                         1.47900E-01 0.2165
  3he(3he-1) .... (3he-3)/4!
                                1.87750E-01 0.5063
                                                         1.87750E-01 0.5063
  3he(3he-1) .... (3he-4)/5! 2.96500E-01 0.7493
                                                         2.96500E-01 0.7493
  3he(3he-1) .... (3he-5)/6! 4.61900E-01 0.8727
3he(3he-1) .... (3he-6)/7! 6.15800E-01 0.9311
                                                         4.61900E-01 0.8727
                                                        6.15800E-01 0.9311
  3he(3he-1) .... (3he-7)/8! 6.68950E-01 0.9626
                                                       6.68950E-01 0.9626
                                5.83050E-01 0.9812
4.03700E-01 0.9918
  3he(3he-1) .... (3he-8)/9!
                                                         5.83050E-01 0.9812
  3he(3he-1) .... (3he-9)/10!
                                                         4.03700E-01 0.9918
  3he(3he-1) .... (3he-10)/11! 2.19000E-01 0.9972
                                                         2.19000E-01 0.9972
  3he(3he-1) .... (3he-11)/12! 9.10500E-02 0.9994
                                                         9.10500E-02 0.9994
```

### Example 2: Infinite Gate

```
Input:
```

```
f38:n 22
ft38 cap 2003 gate 0 1e11
```

### Output:

```
neutron captures, moments and multiplicity distributions. tally
                                                                                          38
print table 118
 weight normalization by source histories =
                                                        20000
 cell:
          22
neutron captures on 3he
 time gate: predelay = 0.0000E+00
                                        gate width = 1.0000E+11
                                                          pulse fraction
                    occurrences occurrences
    in gate histogram by number
                                    by weight
                                                    by number
                                                                 by weight
                                                                                 error
                  6552
                                   0.00000E+00
                                                                3.27600E-01
 captures = 0
                             0
                                                  3.27600E-01
                                                                                0.0101
 captures = 1
                  1002
                          1002
                                   5.01000E-02
                                                  5.01000E-02
                                                                5.01000E-02
                                                                                0.0308
 captures = 2
captures = 3
                                                                2.07000E-02
                                   4.14000E-02
                                                  2.07000E-02
                   414
                           828
                                                                                0.0486
                   176
                           528
                                   2.64000E-02
                                                  8.80000E-03
                                                                 8.80000E-03
                                                                                0.0750
 captures = 4
                                  1.64000E-02
                                                  4.10000E-03
                   82
                           328
                                                                4.10000E-03
                                                                                0.1102
                        210
96
 captures = 5
                                  1.05000E-02
                   42
                                                  2.10000E-03
                                                                2.10000E-03
                                                                                0.1541
                  42
16
8
3
2
2
2
1
 captures =
             6
                           96
56
                                   4.80000E-03
                                                  8.00000E-04
                                                                8.00000E-04
                                                                                0.2499
 captures = 7
                                  2.80000E-03
                                                  4.00000E-04
                                                                4.00000E-04
                                                                                0.3535
 captures = 8
                           24
                                  1.20000E-03
                                                  1.50000E-04
                                                                1.50000E-04
                                                                                0.5773
 captures = 9
                           18
20
                                  9.00000E-04
                                                  1.00000E-04
                                                                1.00000E-04
                                                                                0.7071
 captures = 10
                                  1.00000E-03
                                                  1.00000E-04
                                                                 1.00000E-04
                                                                                0.7071
                          22
12
13
 captures = 11
                                  1.10000E-03
                                                  1.00000E-04
                                                                1.00000E-04
                                                                                0.7071
 captures = 12
                                  6.00000E-04
                                                  5.00000E-05
                                                                5.00000E-05
                                                                                1.0000
 captures = 13
                                  6.50000E-04
                                                  5.00000E-05
                                                                 5.00000E-05
                                                                                1.0000
                           14
                                  7.00000E-04
                                                  5.00000E-05
                                                                 5.00000E-05
 captures = 14
                                                                                1.0000
                     1
 captures = 15
                                  7.50000E-04
                           15
                                                  5.00000E-05
                                                                5.00000E-05
                                                                               1.0000
    total
                  8305
                          3186
                                  1.59300E-01
                                                                 4.15250E-01
                                                  4.15250E-01
                                                                                0.0291
      factorial moments
                                       by number
                                                                by weight
                                 1.59300E-01 0.0651
                                                           1.59300E-01 0.0648
          n(n-1)/2!
                                  1.47900E-01 0.2165
                                                           1.47900E-01 0.2165
        n(n-1)(n-2)/3!
                                  1.87750E-01 0.5063
                                                           1.87750E-01 0.5062
    n(n-1)(n-2) \dots (n-3)/4!
                                                           2.96500E-01 0.7492
                                 2.96500E-01 0.7493
    n(n-1)(n-2) \dots (n-4)/5!
                                 4.61900E-01 0.8727
                                                           4.61900E-01 0.8726
   n(n-1)(n-2) \dots (n-5)/6!

n(n-1)(n-2) \dots (n-6)/7!

n(n-1)(n-2) \dots (n-7)/8!
                                 6.15800E-01 0.9311
                                                           6.15800E-01 0.9311
                                 6.68950E-01 0.9626
                                                           6.68950E-01 0.9626
                                 5.83050E-01 0.9812
                                                           5.83050E-01 0.9812
    n(n-1)(n-2) \dots (n-8)/9!
                                 4.03700E-01 0.9918
                                                           4.03700E-01 0.9918
    n(n-1)(n-2) ... (n-9)/10! 2.19000E-01 0.9972 n(n-1)(n-2) ... (n-10)/11! 9.10500E-02 0.9994 n(n-1)(n-2) ... (n-11)/12! 2.80000E-02 1.0000
                                                           2.19000E-01 0.9972
                                                           9.10500E-02 0.9994
                                                           2.80000E-02 1.0000
```

# Example 3: Finite Gate

#### Input:

```
f78:n 22
ft78 cap gate .5 .4 -40 -40 2003
```

### Output:

```
neutron
             captures,
                         moments and multiplicity distributions.
                                                                           tally
                                                                                      78
print table 118
weight normalization by source histories =
                                                     20000
cell:
          22
neutron captures on 3he
time gate: predelay = 5.0000E-01
                                        gate width = 4.0000E-01
                    occurrences occurrences
                                                       pulse fraction
    in gate histogram by number
                                                               by weight
                                   by weight
                                                 by number
                                                                             error
                 7837
                           Ω
                                 0.00000E+00
                                               3.91850E-01
                                                             3.91850E-01
                                                                            0.0118
 captures =
                          394
                                 1.97000E-02
                                                             1.97000E-02
 captures =
             1
                  394
                                               1.97000E-02
                                                                            0.0666
                          134
                                 6.70000E-03
                                               3.35000E-03
                                                              3.35000E-03
 captures =
             2
                   67
                                                                            0.1542
                                 9.00000E-04
                                               3.00000E-04
                                                              3.00000E-04
captures =
             3
                    6
                           18
                                                                            0.4082
 captures =
                                 2.00000E-04
                                               5.00000E-05
                                                              5.00000E-05
                                                                            1.0000
 total
                 8305
                          550
                                 2.75000E-02
                                               4.15250E-01
                                                              4.15250E-01
                                                                            0.0624
     factorial moments
                                    by number
                                                            by weight
                                2.75000E-02 0.0717
                                                         2.75000E-02 0.0716
          n(n-1)/2!
                                4.55000E-03 0.1654
                                                         4.55000E-03 0.1654
        n(n-1)(n-2)/3!
                                                         5.00000E-04 0.4690
                                5.00000E-04 0.4690
                                5.00000E-05 1.0000
   n(n-1)(n-2) \dots (n-3)/4!
                                                         5.00000E-05 1.0000
```

Scratch space is needed to save capture times during the course of a history. The times are stored temporarily in the capture and moment bins of the tally. If insufficient bins are available, then the number of allowed captures and moments must be increased using the negative entries after the "cap" keyword. The message "\*\*\* warning \*\*\* dimension overflow. Some pulses not counted." is put in Print Table 118 if the space needs to be increased.

## 3.3. User Specification of Multiplicity Constants—FMULT

A new MCNPX input card, FMULT, enables users to override or add new fission multiplicity data as

**FMULT** 
$$ZAID$$
 [ keyword = values ] ,

Where the keywords are

74.75	
ZAID =	nuclide for which data are entered.
SFnu =	average v for sampling spontaneous fission multiplicity from a Gaussian distribution with <i>Width</i> ; or
=	cumulative probability of spontaneous fission multiplicity.
	SFnu is used for spontaneous fission only; for induced fission, v is taken
	from the nuclear data library at the energy of the incident neutron.
Width =	Gaussian width for sampling v for both spontaneous and induced fission,
	ignored for spontaneous fission when SFnu is specified as a cumulative
	probability distribution.
SFYield =	spontaneous fission yield ( n/s-g )—used for selecting the spontaneous

fission nuclide when more than one is present in a material.

Wat = watt energy spectrum parameters a and b for spontaneous fission neutron energy sampling. Induced fission energies are sampled from the nuclear data library.

ZAID must be specified. Defaults exist only for the most common fission nuclei; these defaults are provided in Print Table 38 of the MCNPX output. Width is used for both spontaneous and induced fission; SFYield is used only for spontaneous fission. SFnu and Watt are used only for spontaneous fission; for induced fission, the values are sampled from the nuclear data library.

## Examples:

```
FMULT 98252 SFYield = 2.34e12 SFnu = .002 .028 .155 .428 .732 .917 .983 .998 1. Width = 1.207 Watt = 1.18 1.03419

FMULT 94239 Watt = .885247 3.8026 Width = 1.14 SFYield = .0218 SFnu = 2.16
```

All values are printed in the MCNPX output file in Print Table 38. The data in Table 1 are the default values in MCNPX, not the values modified with the FMULT cards above.

## 3.3.1. New Spontaneous Fission Multiplicity Data

New spontaneous fission multiplicity data are now available in MCNPX and are shown in Table 1. The new data are all the tabular spontaneous fission v values, "sfnu"; the widths, spectra, and yields are unchanged. The new default values\* have been obtained from Battelle Northwest Laboratory and other sources modified by Peter Santi.† The spontaneous fission multiplicity table values are printed in Print Table 38 to only three-digit accuracy but are accurate to seven digits in MCNPX.

Table 1. MCNPX Output File Print Table 38 Displaying Fission Multiplicity Data

1fission multiplicity data. print table 38 zaid width watt1 watt2 yield sfnu .800000 4.00000 6.00E-08 90232 1.079 2.140 1.079 .892204 1.30E+00 92232 3.72278 1.710 92233 .854803 4.03210 8.60E-04 1.760 1.041 1.079 .771241 4.92449 5.02E-03 92234 1.810 2.99E-04 92235 1.072 .774713 4.85231 1.860 92236 1.079 .735166 5.35746 5.49E-03 1.910 .648318 1.36E-02 .297 .722 .950 .993 1.00 1.00 1.00 1.00 1. 92238 1.230 6.81057 0.048 1.079 1.14E-04 93237 2.050 . 833438 4.24147 .670 .293 .905 .980 0.000 0.00E+00 1.00 1.00 1.00 1.00 1. 94236 .000000 0.00000 0.080 .847833 .974 94238 1.115 4.16933 2.59E+03 0.056 .267 .647 .869 1.00 1.00 1.00 1.00 1. .885247 2.18E-02 94239 1.140 3.80269 2.160 94240 1.109 .794930 4.68927 1.02E+03 0.063 .295 .628 .881 .980 .998 1.00 1.00 1.00 1. 1.079 .842472 4.15150 5.00E-02 2.250

\* John S. Hendricks, "New Spontaneous Fission Data,", Los Alamos National Laboratory internal memoranda D-5:JSH-2005-064 (December 14, 2004).

<sup>&</sup>lt;sup>†</sup> P. Santi, D. Beddingford, and D. Mayo, "Revised Prompt Neutron Emission Multiplicity Distributions for 236,238-Pu," Los Alamos National Laboratory report LA-UR-04-8040 (December 2004).

```
.819150
 94242 1.069
                         4.36668
                                   1.72E+03
                                              0.068
                                                      .297
                                                             .631
                                                                   .879
                                                                          .979
                                                                                .997
                                                                                      1.00 1.00 1.00 1.
 95241
        1.079
                .933020
                         3.46195
                                   1.18E+00
                                              3.220
                                                             .495
                                                                                       .999
96242
        1.053
                .887353
                         3.89176
                                   2.10E+07
                                                      .168
                                                                   .822
                                                                          .959
                                                                                .996
                                                                                             1.00
                                                                                                    1.00 1.
                                              0.021
 96244
        1.036
                .902523
                          3.72033
                                   1.08E+07
                                              0.015
                                                      .131
                                                             .431
                                                                   .764
                                                                          .948
                                                                                .991
                                                                                       1.00
                                                                                             1.00
                                                                                                    1.00
 96246
        0.000
                .000000
                          0.00000
                                   0.00E+00
                                              0.015
                                                      .091
                                                             .354
                                                                   .699
                                                                          .917
                                                                                .993
                                                                                       1.00
                                                                                             1.00
                                                                                                    1.00 1.
 96248
        0.000
                .000000
                          0.00000
                                   0.00E+00
                                              0.007
                                                      .066
                                                             .287
                                                                   .638
                                                                          .892
                                                                                .982
                                                                                       .998
                                                                                             1.00
                                                                                                    1.00 1.
        1.079
                .891281
                          3.79405
                                   1.00E+05
                                              3.400
                                                             .349
                                                                   .623
                                                                          .844
                                                                                .970
                                                                                       1.00
                                                                                             1.00
                                                                                                    1.00 1.
 98246
        0.000
                .000000
                          0.00000
                                   0.00E+00
                                              0.001
                                                      .114
                                                             .208
 98250
        0.000
                .000000
                          0.00000
                                   0.00E+00
                                              0.004
                                                      .040
                                                                   .502
                                                                          .801
                                                                                .946
                                                                                       .993
                                                                                             .997
                                                                                                    1.00 1.
 98252
        1.207 1.180000
                          1.03419
                                   2.34E+12
                                              0.002
                                                      .028
                                                             .153
                                                                   .427
                                                                          .733
                                                                                .918
                                                                                       .984
                                                                                             .998
                                                                                                    1.00
                .000000
                                                                                       .983
                                                                                             .998
 98254
        0.000
                          0.00000
                                   0.00E+00
                                              0.000
                                                      .019
                                                             .132
                                                                   .396
                                                                         .714
                                                                                .908
                                                                                                    1.00 1.
100257
        0.000
                .000000
                          0.00000
                                   0.00E+00
                                              0.021
                                                      .073
                                                             .190
                                                                   .390
                                                                          .652
                                                                                .853
                                                                                       .959
                                                                                             .993
                                                                                                    1.00 1.
                                   0.00E+00
                                                                                .717
        0.000
                .000000
                          0.00000
                                              0.057
                                                             .207
                                                                   .351
                                                                          .534
                                                                                             .959
                                                                                                    .997 1.
102252
                                                      .115
                                                                                       .863
```

All of the available data are printed when Print Table 38 is turned on by the **PRINT** card. Data actually used are denoted by "\*". If any data are overridden by FMULT user input, the user data replaces the default data shown in Print Table 38.

Tracking MCNPX 25e data:

MCNPX Version 2.5.e results can be tracked using the previous set of spontaneous fission multiplicity data by adding the following card to the input deck in MCNPX 2.5.f and later:

The 20J means jump over the 1<sup>st</sup> 20 entries on the DBCN card. The 21<sup>st</sup> entry causes MCNPX 25f to track MCNPX 25e. If the 21<sup>st</sup> entry is 1, then all changes from MCNPX 25e are undone, including some bug corrections. If the 21<sup>st</sup> entry is -1, then only the spontaneous fission multiplicity data changes are undone.

Thus, users performing a series of calculations with the old data can continue to use it by adjusting tracking with the DBCN card and using DBCN(21) = -1 as above.

Nuclides without transport cross sections:

MCNP(X) does not provide nuclear cross sections for transporting Cf-246, Cf-254, Fm-257, and No-252.

To model spontaneous fission from these nuclides, it is necessary to do the transport either with a physics model or by substituting cross sections. Physics models are not recommended at fission energies. To make a nuclide substitution, use the AWTAB and MX cards. For example:

M123	100257	1.
AWTAB	100257	257.
MX123:N	98252	

The AWTAB card provides the atomic weight ratio for Fm-257, which is not provided in the standard MCNP(X) data libraries. The MX123:N card substitutes Cf-252, for which there is neutron cross section data, for the corresponding nuclide (100257) on the M123 materials card.

Nuclides without multiplicity data:

<sup>\* =</sup> used in problem.

Fission widths, watt fission spectra parameters, and fission yields are not available for the above nuclides, which do not have transport cross sections: Cf-246, Cf-254, Fm-257, and No-252. They are also not available for Pu-246, Cm-246, Cm-248, and Cf-250. Note that the values for width, watt1, watt2 and yield in print table 38 (above) are all zero for these eight nuclides. To have a spontaneous fission source for these nuclides, an FMULT input file data card is required. For example,

FMULT 96246 width=1.1 watt=.2 4 sfyield 1 .

Because the multiplicities are provided as a table with 10 bins, the width is ignored for the spontaneous fission source but a value is still required for induced fission. For spontaneous fission, the energy distribution is sampled from the two Watt-fission spectra parameters; for induced fission, the energy spectra is chosen from parameters in the nuclear data tables of the transport cross sections. Finally, the spontaneous fission yield must be specified if there is more than one spontaneous fission source nuclide. The yield is used to determine the relative sampling between spontaneous fission source nuclides. These parameters have no default values; if the FMULT card is missing, a fatal error message is issued:

fmult card needed for za = 96246.

# 3.4. Correct for Fission Multiplicity Negative Gaussian Tail Bias

When fission multiplicity is specified on the PHYS:N card, the number of fission neutrons, v, is sampled from a Gaussian distribution. Because negative neutrons are not allowed, whenever they are sampled, zero, rather than negative numbers of neutrons are produced. Consequently, the average sampled value of v is biased above what it should be.

The negative Gaussian bias for fission multiplicity has been corrected.\* When fission multiplicity is turned on for induced fission and for spontaneous fission, the number of fission neutrons, v, is sampled from a Gaussian distribution when a cumulative multiplicity distribution is not available. A small correction is made to each sampled v value to preserve the first moment, the average number of neutrons per fission. The specification of fission multiplicity has been changed:

**PHYS**:N 5J fissmult,

where

fissmult = 0: no fission multiplicity: MCNP method—sample v from nearest integer which preserves the first moment but gives incorrect multiplicity;

<sup>\*</sup> John S. Hendricks, "Monte Carlo Sampling of Fission Multiplicity," Los Alamos National Laboratory report LA-UR-04-6967, submitted to Monte Carlo 2005, Chattanooga, TN (April 17–21, 2005).

- = 1 : correct sampled v to preserve the first moment (recommended);
- = 2 : preserve first moment by increasing v threshold.
- = 3 : old MCNPX 2.5.e method—uncorrected fission multiplicity;
- = 4 : MCNP method in presence of spontaneous fission or FMULT card.

*Defaults:* If an FMULT card is present or if a spontaneous fission source is used (par = sf on SDEF card), then the default is fissmult = 1; otherwise, the default is fissmult = 0.

If fissmult = -1 (MCNPX 2.5.E specification), it is changed to +1 for backward compatibility. To specify a width for fission multiplicity (fissmult > 0 in MCNPX 2.5.E), the **FMULT** card must be used.

The effect of the negative Gaussian bias correction is small unless the fission multiplicity width approaches the value of v. The example below compares the new default spontaneous fission multiplicity data for Pu-236 ("table") with artificially distorted Gaussian distributions with the above four options:

```
"Gauss c1" fissmult = 1 Gaussian with correction 1
"Gauss c2" fissmult = 2 Gaussian with correction 2
"Gaussian" fissmult = 3 uncorrected Gaussian (MCNPX 25e)
"MCNP4C" fissmult = 4 MCNP4C nearest integer method
```

As expected, the MCNP4c method fails to represent the spontaneous fission multiplicity, which is the correct "table" value. The Gaussian values are fictitiously broadened by artificially setting the width = 2, which is nearly the  $\nu$  value of 2.07 for Pu-236. Correction 1 shifts the multiplicity lower to preserve the average  $\nu$  value. Correction 2 increases multiplicity 0 at the expense of multiplicity 1 to preserve the average  $\nu$  value. The uncorrected Gaussian distribution has the true Gaussian shape centered about  $\nu$ , but the average  $\nu$  value is biased to 2.2249 instead of 2.07. Certainly, with realistic values of the width, these differences are very small.

## 3.5. Translated Sources Can Have Dependence

MCNPX allows translating sources to different locations with the TR option on the SDEF card. This capability is most useful for setting up the source as an accelerator beam and then using the translation as a distribution to repeat the accelerator source at different locations and orientations.

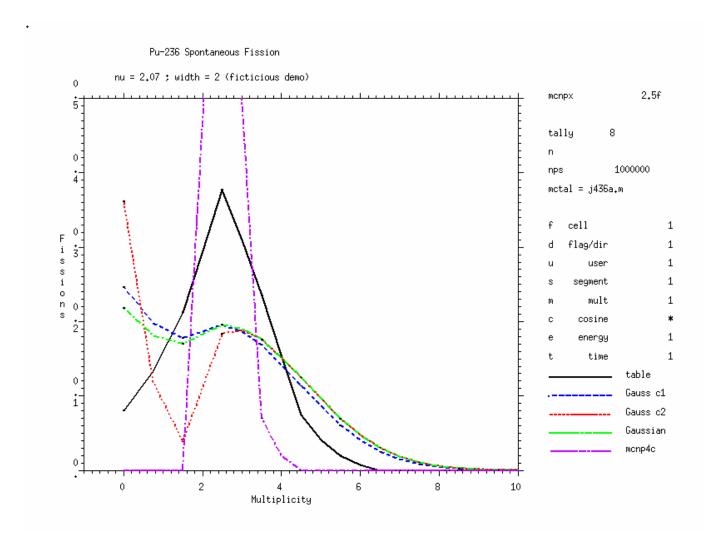
The TR option on the SDEF card now can be dependent on other source variables. For example, the particle type can depend on the translated source location:

```
SDEF CEL=FTR=D3 PAR=FTR=D1 TR=D2.
```

Or the translated source location can be a dependent distribution function of cell:

```
SDEF CEL=D2 TR=FCEL=D5.
```

Thus, the TR parameter on the SDEF card is more consistent with the other source parameters.



Note that TR must be sampled before POS and the cookie-cutter checks (CCC) parameter. For backward compatibility, the source translation (TR) is performed only after the CCC rejection when TR is an explicit value or an independent distribution.

## 3.6. Plot Pause Command Interrupts

MCNP(X) allows plots to be made from command files: MCNPX IP COM=command\_filename or MCNPX Z COM=command\_filename. The command\_filename file contains plot commands that also can use the plot pause command to stop either for a specified amount of time (to make slide shows) or until the user strikes a key. Users can now interrupt the reading of the command files and return control of plotting to the terminal by entering "quit." After each picture is displayed, the message to the command terminal is now

Strike any key to continue. Quit returns to interactive mode.

## 3.7. PTRAC for N-Particles

The PTRAK capability of writing particle tracks to a file for postprocessing has been extended to include all particle types and has provided appropriate information for all model collision/bank events.

## 3.8. DXTRAN/Detectors with Model Physics (Isotropic Approximation)

All collisions producing neutrons and photons now contribute to DXTRAN and point detectors, including model physics interactions. When the secondary neutron/photon angular scattering distribution function is unknown (generally the case for model physics), isotropic scattering is assumed (poor approximation). Although the extension to higher-energies often thus is approximate, energy bins for the point detector tally can identify what portion of the tally is coming from high energies. Further, this new approximation is superior to neglecting charged-particle and high-energy neutron collisions altogether [previous MCNP(X) versions].

### 3.9. Additional Enhancements

The following enhancements were made to MCNPX 2.5.f, in addition to the major new capabilities explained in Section 2.0.

## **3.9.1.** Autoconfiguration Enhancements

The MCNPX autoconfiguration installation package was upgraded to be more consistent with Fortran90, including Linux Intel compilers (and test set templates). (TLR)

## 3.9.2. Computer Time Accuracy

Computer time used (CTM) is now rounded up to 1e-6 s, not 1 s, thus improving the comparison of code timing. (GWM)

### 3.9.3. Cleanup Search for Cross-Section Data

Cross sections and auxiliary data are now found consistently for MCNPX, HTAPE3X, XSEX3, INCL4, CEM2k, and all parts of MCNPX. The improvement is invisible to users. (LSW)

### 3.9.4. Extend LCS Deexcitation to A = 254

The deexcitation routines (PHT) in the Lahet Code System (LCS) portion of MCNPX have been extended from nuclides with A=250 to A=254. The parameter values for A=250 were approximated as the values for A>250. Before the extension, spurious errors would occur. In particular, Matt Kinlaw (Idaho State University) reported that a crash occurred when a neutron above 20 MeV went to the model physics to interact with Cf-252 (his source material). A pointer went off the end of the PHT table, causing a negative square root crash. (GWM)

### 3.9.5. Resample INCL4 Strange Remnants

If remnants are produced with atomic number Z = A or Z = 0, then interactions are now resampled (INCL4 model only). (JCD)

### 3.9.6. Increase MPI Buffer Limit

The buffer size for MPI parallel processing has been increased to 40MB. (GWM)

### 3.9.7. Reduce Photonuclear Threshold to 1 MeV

The threshold energy for physics model photonuclear reactions is now 1 MeV. For table photonuclear data, it is whatever value is in the table. (GWM)

## 4.0. MCNPX 2.5.<u>f</u> CORRECTIONS

## **4.1.** Significant Problem Corrections

The following problems could cause incorrect answers. Fortunately, they occur only in very special situations and affect only a few MCNPX users.

## 4.1.1. Secondary Particles in DXTRAN Spheres

The check for secondary particles being produced inside DXTRAN spheres has been corrected. The error affected problems with DXTRAN and more than one particle type and affected all previous MCNPX and MCNP versions. (TEB/JSH)

### 4.1.2. DXTRAN/Detectors with Photonuclear or Proton Physics

The use of DXTRAN or point detectors gave erroneous answers in the following cases:

- photon DXTRAN/detectors with photonuclear data table physics;
- any particle DXTRAN/detector with photonuclear model physics; and
- DXTRAN with proton table physics.

Note that DXTRAN/detectors have never worked for (1) secondary neutrons or photons from model physics collisions or (2) primary neutrons in model physics collisions. These now work with an isotropic approximation described in the MCNPX extensions section above.

Use of photon DXTRAN/detectors caused incorrect photonuclear table physics results. The table physics cross sections used for the DXTRAN/detector pseudo-particles were not reset back to the appropriate values for further transport of continuing or subsequent secondary particles. Consequently, both subsequent secondary photonuclear particles and subsequent photoatomic interactions used the wrong cross sections (KTC/RTC arrays) and gave incorrect answers.

Use of photon or neutron DXTRAN/detectors with photonuclear model physics resulted in erroneous photoatomic sampling. The total cross section saved (TOTM) for transport after DXTRAN/detectors failed to include a reduction for the model contribution (TOTPNC).

Use of photon DXTRAN with proton transport resulted in erroneous neutron DXTRAN contributions—even in the table physics library energy regime. The flag (IDX) identifying whether the photon was in a DXTRAN sphere was improperly set.

Paul Goldhagen, EML/USDHS, New York, first reported these MCNP carryover problems and was awarded \$2 (D-5:JSH-2005-091). (GWM)

## **4.1.3.** Bremsstrahlung Angular Distributions

Bremsstrahlung angular distributions could be wrong in all previous MCNP and MCNPX versions. The bug involved an out-of-bounds reference that caused the MACG5 to crash. Most systems just used the bogus data and continued. Whenever the electron energy was within the last few energy bins (near the cutoff), the logic in the bremsstrahlung (subroutine brems) angular distribution would result in a reference to arrays eee or ech that extracted values for the wrong material or extracted bogus values from an out-of-bounds index. Now the faulty reference is corrected by using the "simple model" for angular distributions when the out-of-bounds reference happens. \$2 was awarded to Paul Bailey, DOE/EML, Argonne, IL (D-5:JSH-2004-044). (GWM)

## **4.1.4.** Delayed Neutron Fission Multiplicity

The combination of analog delayed neutron production with fission multiplicity (PHYS:N 3J -1 J -1) would not terminate the continuing neutron when the fission multiplicity was sampled as zero (rare case). €20 was awarded Steven van der Marck, NRG, Petten, Netherlands (D-5:JSH-2004-084). (GWM)

## **4.1.5.** Surface Sources with Antiparticles

Antiparticles were not properly written to surface sources because the antiparticle flag was set inconsistently. \$20 was awarded to Falk Poenisch, M. D. Anderson Cancer Treatment Center, Houston (D-5:JSH-2004-101). (GWM)

## **4.1.6.** Pulse-Height Tallies in Repeated Structures

PHTs have always worked when the PHT cell was at the lowest level (the transported particle level). But PHTs have never worked for PHTs specified in repeated structures cells filled with cells at a lower level. This has been corrected. \$2 was awarded Valery Taranenko, GSF, Germany (D-5:JSH-2004-102). (GWM)

# 4.1.7. Photonuclear Tally Multipliers

Photonuclear FM tallies fail when the FM tally multiplier material is not the same material as the one in the tallying cell. In these cases, the code loads the tally material to make the FM tally but fails to reset some material-related parameters when transport in the tally cell is resumed using the cell material. \$20 was awarded to Brad Micklich, ANL (D-5:JSH-2004-145). (GWM)

### 4.2. Minor Problem Corrections

The following problems do not cause wrong answers, but they may cause crashes when encountered. In any case, they occur only in very special situations and affect only a few MCNPX users.

#### $4.2.1. \qquad SDEF Par = d$

Specification of deuteron sources, SDEF Par=d, failed because the "d" was interpreted as a distribution when MCNPX 2.5.e added the capability of multiple source particles. €20 was awarded to Laurent Bourgois, CEA, Saclay, France (D-5:JSH-2004-036). (JSH)

### 4.2.2. AIX / MPI 8-Byte Integers

The 8-byte integer capability now works with MPI for all operating systems. (GWM)

### 4.2.3. KCODE Mode D Crash

A KCODE problem with lattices, print table 128, and Mode "n d" crashed because the universe map cannot be written with particle types > 3. \$2 was awarded Tak Pui Lou, LBL (D-5:JSH-2004-137) (JSH)

### **4.2.4. PTRAC Reaction Numbers**

PTRAC did not print the correct reaction number in some cases for photon interactions. \$2 was awarded Caroline Boudou, INSERM, Grenoble, France. (D-5:JSH-2004-138) (GWM)

### 4.2.5. New NJOY Fission Data Problem

Nuclear cross-section data for some fissionable nuclides generated with some new versions of NJOY have a negative reaction type flag. The flag, NTYN = -19, signifies fission secondaries described in the center-of-mass (COM) reference frame using scattering Law 44 Kalbach-87. This does not affect KCODE problems or fixed source problems without NONO. It does not apply to any nuclear data currently distributed with MCNP(X). \$2 was awarded Steven van der Marck, NRG, Netherlands (D-5:JSH-2005-45). (GWM)

## 4.2.6. Error Trap and Remedy for Too Many Duplicate Surfaces

If a macrobody surface specification results in more than 93 duplicate surfaces that are deleted, MCNP(X) overflows some arrays causing serious problems. Now if the duplicate surface arrays overflow, a fatal error message, "overflow of duplicate surface array, increase mnds." occurs. Either the geometry can be corrected to have fewer duplicate surfaces or the value of the mnds parameter can be increased from its present value of 100. This enhancement was suggested by W. Bernnat, IKE University of Stuttgart, Germany. (GWM).

### **4.2.7. Default Cosine Bins for Surface Flux Tallies**

The cosine default on the C0 card now apply to F2 surface flux tallies. \$2 was awarded Fan Lei, QinetiQ, Farnborough, UK (D-5:JSH-2005-092). (GWM)

## 5.0. FUTURE WORK

The following projects are at least partially funded and are actively being developed. These capabilities should be available soon in a future MCNPX version.

- Cinder90 capabilities
  - Delayed neutrons physics models
  - Delayed gamma physics models
  - Transmutation
- Criticality
  - Externally driven sources
  - Improved stability of eigenfunctions
- Improved high-energy physics with the LAQGSM model
- Integration of HTAPE tallies directly into MCNPX, including continue runs
- Heavy-ion tracking and interactions
- Electric and magnetic field tracking

The following projects are on our wish list. Some have been partially developed but await further funding.

- detectors and DXTRAN for all neutral particles at all energy ranges with anisotropic scattering (presently approximated as isotropic for models),
- CAD link,
- secondary particle angle biasing for isotropic distributions,
- neutral particle perturbation techniques extended to physics model region,
- plotting of physics model total and absorption cross sections, and
- forced collisions for neutral particles extended to physics models.